Materials Science

MOLECULAR MODELING OF DEFECT STRUCTURES IN PENTACENE

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Pentacene is a crystalline organic material that has shown promise for use in applications such as thin film transistors. We performed simulations to calculate surface energies for the low index crystallographic faces, and it was found that the (001) surface had the lowest energy at 50 mJ/m^2. Next we calculated the dislocation energies for dislocations of varying Burgers vector and density. Using this data, we were able to determine the relationship between system energy and defect density. Also, using the dislocation energies, we were able to calculate defect energies for low angle grain boundaries. Finally, we have modeled low angle grain boundaries by building (100)//(n01) interfaces. We have seen (001) plane bending in these simulations, as well as the splitting of edge dislocations into partial dislocations, which allow for the accommodation of the defect.